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LOGINID:ssspta1611sxp

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	Apr 08	"Ask CAS" for self-help around the clock
NEWS	3	Jun 03	New e-mail delivery for search results now available
NEWS	4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS	5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS	6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS	7	Sep 03	JAPIO has been reloaded and enhanced
NEWS	8	Sep 16	Experimental properties added to the REGISTRY file
NEWS	9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS	10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS	11	Oct 24	BEILSTEIN adds new search fields
NEWS	12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS	13	Nov 18	DKILIT has been renamed APOLLIT
NEWS	14	Nov 25	More calculated properties added to REGISTRY
NEWS	15	Dec 04	CSA files on STN
NEWS	16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS	17	Dec 17	TOXCENTER enhanced with additional content
NEWS	18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS	19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS	20	Feb 13	CANCERLIT is no longer being updated
NEWS	21	Feb 24	METADEX enhancements
NEWS	22	Feb 24	PCTGEN now available on STN
NEWS	23	Feb 24	TEMA now available on STN
NEWS	24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS	25	Feb 26	PCTFULL now contains images
NEWS	26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS	27	Mar 19	APOLLIT offering free connect time in April 2003
NEWS	28	Mar 20	EVENTLINE will be removed from STN
NEWS	29	Mar 24	PATDPAFULL now available on STN
NEWS	30	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS	31	Apr 11	Display formats in DGENE enhanced
NEWS	32	Apr 14	MEDLINE Reload
NEWS	33	Apr 17	Polymer searching in REGISTRY enhanced
NEWS	34	Apr 21	Indexing from 1947 to 1956 being added to records in CA/CAPLUS
NEWS	35	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS	36	Apr 28	RDISCLOSURE now available on STN

NEWS EXPRESS	April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
NEWS HOURS	STN Operating Hours Plus Help Desk Availability

Patel <5/3//2003>

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 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *



FILE 'HOME' ENTERED AT 10:43:28 ON 03 MAY 2003

=> ile reg
ILE IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                   0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:43:42 ON 03 MAY 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     2 MAY 2003  HIGHEST RN 509953-09-7
DICTIONARY FILE UPDATES:    2 MAY 2003  HIGHEST RN 509953-09-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
```

conducting SmartSELECT searches.

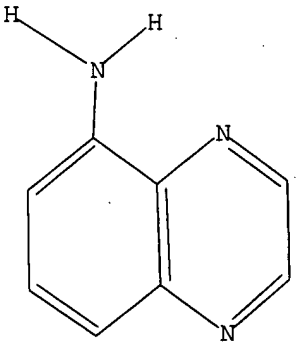
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10077150.2

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:43:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 298 TO ITERATE

100.0% PROCESSED 298 ITERATIONS 19 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4925 TO 6995
PROJECTED ANSWERS: 119 TO 641

L2 19 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:44:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5624 TO ITERATE

100.0% PROCESSED 5624 ITERATIONS 311 ANSWERS
SEARCH TIME: 00.00.01

L3 311 SEA SSS FUL L1

```
=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   148.15     148.36

FILE 'CAPLUS' ENTERED AT 10:44:12 ON 03 MAY 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 3 May 2003  VOL 138 ISS 19
FILE LAST UPDATED: 2 May 2003  (20030502/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l3
L4          261 L3

=> s l4 and pyrimidine
L5            5 L4 AND PYRIMIDINE

=> s l4 and diaminipyrimidine
L6            0 L4 AND DIAMINIPYRIMIDINE

=> d l5 fbib hitstr abs total

L5   ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2003 ACS
AN   1997:618093  CAPLUS
DN   127:293249
TI   Preparation of quinoxalinediones as NMDA receptor antagonists
IN   Bull, David John; Carr, Christopher Lee; Fray, Michael Jonathan; Gautier,
     Elisabeth Colette Louise; Mowbray, Charles Eric; Stobie, Alan
PA   Pfizer Research and Development Company, N.V., UK; Pfizer Inc.; Bull,
     David John; Carr, Christopher Lee; Fray, Michael Jonathan; Gautier,
     Elisabeth Colette Louise; Mowbray, Charles Eric; Stobie, Alan
SO   PCT Int. Appl., 153 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 2
     PATENT NO.         KIND  DATE          APPLICATION NO.  DATE
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PI   WO 9732873          A1   19970912      WO 1997-EP995    19970227
         W:  AU, BG, BR, CA, CN, CZ, HU, IL, IS, JP, KR, LK, LV, MX, NO, NZ,
             PL, RO, SG, SI, SK, TR, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ,
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MD, RU, TJ, TM
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

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TW 454004	B	20010911	TW 1997-86101412	19970205
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CA 2248366	AA	19970912	CA 1997-2248366	19970227
			GB 1996-5027	A 19960309
AU 9720231	A1	19970922	AU 1997-20231	19970227
AU 717972	B2	20000406		
			GB 1996-5027	A 19960309
			WO 1997-EP995	W 19970227
EP 885212	A1	19981223	EP 1997-908156	19970227
EP 885212	B1	20011114		

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			WO 1997-EP995	W 19970227
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ZA 9701987	A	19980907	ZA 1997-1987	19970307
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				WO 1997-EP995 W 19970227
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	MX 9907937	A	20000731	MX 1999-7937 19990826
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				WO 1998-EP1275 W 19980224

PATENT FAMILY INFORMATION:

FAN 1998:608616

	PATENT NO.	KIND	DATE	APPLICATION NO. DATE
PI	WO 9838186	A1	19980903	WO 1998-EP1275 19980224
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
				GB 1997-15783 A 19970725
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				GB 1997-15783 A 19970725
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	EP 973766	A1	20000126	EP 1998-913660 19980224
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LV, FI, RO			
				WO 1997-CA995 W 19970227
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			WO 1998-EP1275 W 19980224
NO 9904135	A	19991022	NO 1999-4135 19990826
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			WO 1998-EP1275 W 19980224
MX 9907937	A	20000731	MX 1999-7937 19990826
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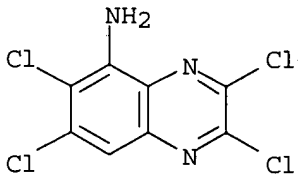
			WO 1998-EP1275 W 19980224

OS MARPAT 127:293249

IT **178619-88-0P 178619-89-1P 178907-46-5P**
178907-47-6P 178907-48-7P 178907-49-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of quinoxalinediones as NMDA receptor antagonists)

RN 178619-88-0 CAPLUS
CN 5-Quinoxalinamine, 2,3,6,7-tetrachloro- (9CI) (CA INDEX NAME)



RN 178619-89-1 CAPLUS
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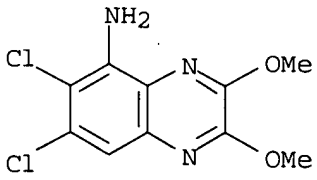

RN 178907-46-5 CAPLUS
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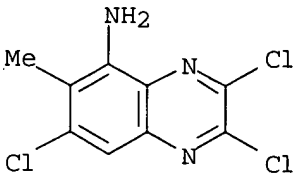

RN 178907-47-6 CAPLUS
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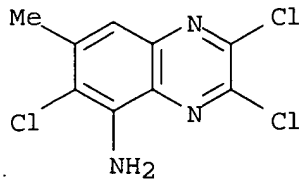

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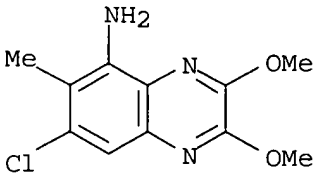

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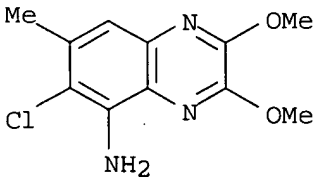
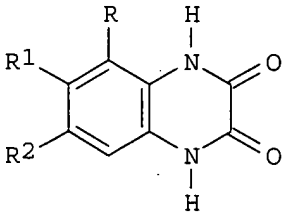


GI

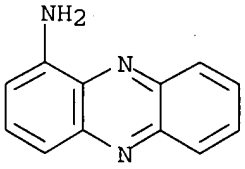


I

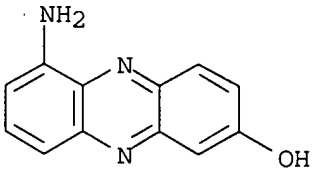
AB The title compds. [I; R = (un)substituted 5-membered heteroaryl contg. 3 or 4 N atoms which is linked to the quinoxalinedione ring by a ring C or N atom, or a 6-membered heteroaryl contg. 1-3 N atoms which is linked to the quinoxalinedione ring by a ring C atom; R1, R2 = H, F, Cl, C1-4 alkyl, etc.], useful as NMDA receptor antagonists for treating acute neurodegenerative and chronic neurol. disorders such as stroke, transient ischemic attack, peri-operative ischemia or traumatic head injury, were prepd. and formulated. Thus, treatment of 6,7-dichloro-2,3-dimethoxy-5-(4-pyridyl)quinoxaline with 2N HCl in 1,4-dioxane afforded 17% I [R = 4-pyridyl; R1 = R2 = H]. Compd. I [R = 1-methyl-1H-tetrazol-5-yl; R1 = R2 = Cl] showed IC50 of 3 nM against binding at the glycine site of the NMDA

receptor.

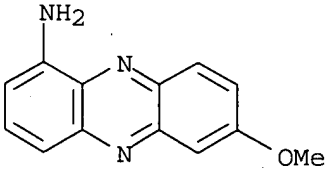
L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS
AN 1963:53246 CAPLUS
DN 58:53246
OREF 58:9060h,9061a-g
TI Phenazines. II. Synthesis of aminophenazines
AU Gaertner, G.; Gray, A.; Holliman, F. G.
CS Univ. Cape Town, S. Afr.
SO Tetrahedron (1962), 18, 1105-14
DT Journal
LA Unavailable
IT **2876-22-4**, Phenazine, 1-amino- **18450-04-9**, 2-Phenazinol, 6-amino- **18450-05-0**, Phenazine, 1-amino-7-methoxy- **92164-56-2**, 2-Phenazinol, 6-amino-, acetate
(prepn. of)
RN 2876-22-4 CAPLUS
CN 1-Phenazinamine (9CI) (CA INDEX NAME)



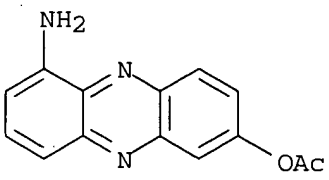
RN 18450-04-9 CAPLUS
CN 2-Phenazinol, 6-amino- (7CI, 8CI) (CA INDEX NAME)



RN 18450-05-0 CAPLUS
CN Phenazine, 1-amino-7-methoxy- (7CI, 8CI) (CA INDEX NAME)



RN 92164-56-2 CAPLUS
CN 2-Phenazinol, 6-amino-, acetate (7CI) (CA INDEX NAME)

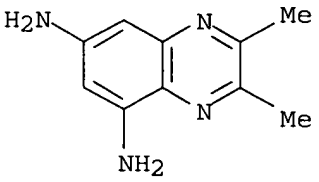


GI For diagram(s), see printed CA Issue.

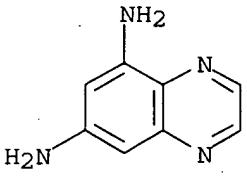
AB Polynitrodiphenylamines (I) were prepd. by Ullmann reactions under a variety of conditions as detailed in tabulation. The appropriate I were catalytically hydrogenated in alc. with prereduced PtO2 or Pd-C at 20-40 lb./sq. in. and the filtered soln. was evapd. (N atm) in vacuo to give the corresponding aminodiphenylamines (II), characterized as the polyacetamido derivs. (R, R1, R2, R3, R4, and m.p. (solvent) given): MeO, AcNH, H, AcNH, H, AcNH, H, 215.0-6.5.degree. (BuOH); H, MeO, AcNH, AcNH, AcNH, H, 238-40.degree. (PhNO2); H, AcNH, MeO, H, AcNH, H, 202-4.degree. (alc.); Me, AcNH, H, H, AcNH, H, 232-4.degree. (dil. alc.); Cl, AcNH, H, H, AcNH, H, 239-41.degree. (dil. alc.). Only II(R = H, R1 = R2 = NH2, R3 = MeO, R4 = H), m. 155-8.degree. (alc.-Norit), was analyzed directly. II (R = MeO, R1 = R3 = R5 = NH2, R2 = R4 = H) from catalytic hydrogenation of 2 g. I in alc. treated with 10 ml. 6N HCl and filtered (N atm.) from catalyst, the filtrate dild. with 6.6 g. FeCl3 in 32 ml. H2O and the mixt. kept 1 day, the alc. evapd. and the residue adjusted to pH 5-6 with NaOAc gave 75% 1-amino-7-methoxyphenazine (III, R = NH2, R3 = MeO, R1 = R2 = R4 = H) (IV), m. 168-71.degree. (ligroine b. 80-100.degree.). IV (0.2 g.) in 4.5 ml. 48% HBr refluxed 3 hrs. and the cooled mixt. made alk., the filtered soln. adjusted to pH 6 with HCl and filtered, the H2O-washed ppt. crystd. from H2O and dried in vacuo over CaCl2 gave III (R = NH2, R3 = OH, R1 = R2 = R4 = H) (V), m. 270.degree. (decompn.), acetylated with Ac2O at 20.degree. to give III (R = NHAc, R3 = OH, R1 = R2 = R4 = H) m. 297.degree. (decompn.). V acetylated at 0.degree. with Ac2O in the presence of aq. NaOH gave III (R1 = AcO, R2 = NH2, R = R3 = R4 = H), m. 182-5.degree. (alc.), hydrolyzed in warm dil. alkali with formation of a deep red soln. V acetylated by heating with Ac2O and NaOAc gave III(R = NHAc, R3 = AcO, R1 = R2 = R4 = H), m. 205-8.degree. (alc.). II obtained from 1 g. of the corresponding nitro compd. refluxed 1 hr. in 50-60 ml. xylene with 15 g. PbO2 and the filtered soln. and washings extd. with 6N HCl, the acid ext. neutralized and the product recrystd. gave the tabulated III (I and III substituents other than H, m.p. III (solvent) and % yield given): R1 = R4 = NO2, R1 = NH2, 274-7.degree. (dil. alc.), -(low); R = R1 = NO2, R1 = NH2, 265-70.degree. (alc.), 13; R1 = R3 = NO2, R1 = NH2, 115-40.degree., -(low); R = R1 = NO2, R4 = MeO, R1 = NH2, R4 = MeO, 212-15.degree. (H2O), -(low); R1 = R2 NO2, R3 = MeO, R = NH2, 169-72.degree. (H2O), 43; R1 = NO2, R = NH2, 169-71.degree. (sublimation), -(low). II (obtained by evapn. of filtered hydrogenation alc. soln.) refluxed 5 hrs. in 25 ml. PhNO2 contg. 0.5 g. m-(O2N)2C6H4 and dild. with 100 ml. 6N HCl, the mixt. steam distd. and the acid residue neutralized gave III (method A). II (catalysts soln. after filtration) dild. with 125 ml. PhNO2 and the alc. evapd., the PhNO2 soln. refluxed 12 hrs. and the soln. concd. in vacuo to 25 ml., the concentrate cooled and filtered yielded III (method B). Phys. data are tabulated (substituents of I other than H, method, substituents of III other than H, m.p. (solvent) and % yield given): R2 = R4 = NO2, R1 = MeO, A,R1 = NH2, R2 = MeO, 278-81.degree. (H2O), 44; R1 = R4 = NO2, A, R1 = NH2, 277-80.degree. (50% alc.), 50; R = R1 = NO2, A, R1 = NH2, 277-80.degree. (50% alc.), 5; R = R1 = NO2, B, R1 = NH2, 270-4.degree. (50% alc.), 50; R = R1 = NO2, R4 = MeO, A, R1 = NH2, R4 = MeO, 216-18.degree. (H2O), 54; R4 = Me, R = R1 = NO2, B,

R1 = NH2, R4 = Me, 228-30.degree. (dil. alc.), 52; R = Me, R1 = R4 = NO2, B, R1 = NH2, R4 = Me, 228-30.degree. (dil. alc.), 46; R = R1 = NO2, R4 = Cl, B, R1 = NH2, R4 = Cl,250-1.degree. (dil. alc.), 45; R = Cl, R1 = R4 = NO2, B, R1 = NH2, R4 = Cl, 247-9.degree. (dil. alc.), 30; R1 = R3 = NO2, A, R = NH2, 174-6.degree. (dil. alc.), 67; R1 = R2 = NO2, A, R = NH2, 174-6.degree. (dil. alc.), 25; R1 = R2 = NO2, R3 = MeO, A, R = NH2, 123-8.degree. (crude, identified by paper chromatography), small. Ultraviolet and visible spectral data, and fluorescence data were given.

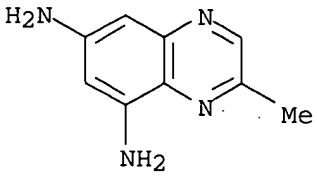
L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2003 ACS
AN 1963:3286 CAPLUS
DN 58:3286
OREF 58:521d-f
TI Polyazanaphthalenes. VII. Some derivatives of quinazoline and 1,3,5-triazanaphthalene
AU Oakes, V.; Rydon, H. N.; Undheim, K.
CS Univ. Exeter, UK
SO J. Chem. Soc. (1962) 4678-85
DT Journal
LA Unavailable
IT **2312-92-7**, Quinoxaline, 5,7-diamino-2,3-dimethyl- **89977-47-9**, Quinoxaline, 5,7-diamino- **90558-60-4**, Quinoxaline, 6,8-diamino-2-methyl- **90558-76-2**, 2-Quinoxalinol, 5,7-diamino-3-methyl- **91769-37-8**, 2-Quinoxalineacetic acid, 6,8-diamino-3-hydroxy-, ethyl ester
(prepn. of)
RN 2312-92-7 CAPLUS
CN 5,7-Quinoxalinediamine, 2,3-dimethyl- (9CI) (CA INDEX NAME)



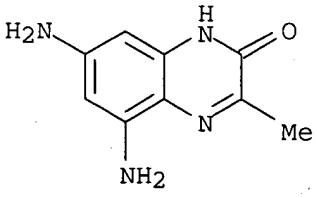
RN 89977-47-9 CAPLUS
CN Quinoxaline, 5,7-diamino- (7CI) (CA INDEX NAME)



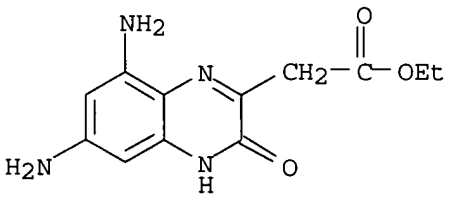
RN 90558-60-4 CAPLUS
CN Quinoxaline, 6,8-diamino-2-methyl- (7CI) (CA INDEX NAME)



RN 90558-76-2 CAPLUS
CN 2-Quinoxalinol, 5,7-diamino-3-methyl- (7CI) (CA INDEX NAME)



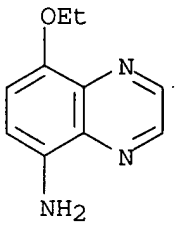
RN 91769-37-8 CAPLUS
CN 2-Quinoxalineacetic acid, 6,8-diamino-3-hydroxy-, ethyl ester (7CI) (CA INDEX NAME)



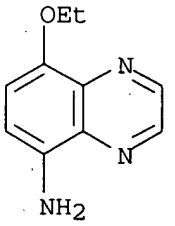
GI For diagram(s), see printed CA Issue.
AB 2,4-Diamino-6-methylquinazoline was synthesized and converted, by side-chain bromination of its dibenzoyl deriv., condensation with ethyl p-aminobenzoatc, and removal of the benzoyl and ester groups, into the pteroic acid analog (I). A similar procedure has led to the successful synthesis of pteroic acid analogs derived from 2,4-diamino- and 2-amino-4-hydroxy-1,3,5-triazanaphthalene. The expected preferential reactivity of the 4-chlorine atom in 2,4-dichloro-6-methylquinazoline is exhibited in its reactions with ammonia, hydrazine, and benzylamine, but not in that with aniline.

L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS
AN 1962:13016 CAPLUS
DN 56:13016
OREF 56:2449d-g
TI 5-Ethoxy-8-aminoquinoxaline
AU Easley, Wm. K.; Monley, Lawrence E.; Hutchins, James E.
CS Northern Louisiana State Coll., Monroe
SO J. Org. Chem. (1961), 26, 3008-9
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
IT **90840-14-5**, Quinoxaline, 5-amino-8-ethoxy- **93439-84-0**,

Quinoxaline, 5-amino-8-ethoxy-, hydrochloride
(prepn. of)
RN 90840-14-5 CAPLUS
CN Quinoxaline, 5-amino-8-ethoxy- (7CI) (CA INDEX NAME)



RN 93439-84-0 CAPLUS
CN Quinoxaline, 5-amino-8-ethoxy-, hydrochloride (7CI) (CA INDEX NAME)

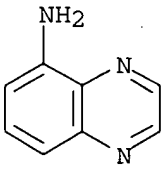


x HCl

AB The synthesis of 5-ethoxy-8-(acetylamino)quinoxa-line (I), 5-ethoxy-8-aminoquinoxaline (II), 5-ethoxy-8-(p-toluenesulfonamido)quinoxaline (III), 5-ethoxy-8-(N-acetyl-sulfanilamido)quinoxaline (IV), and 5-ethoxy-8-sulfanil-amidoquinoxaline (V) was reported together with an im-proved procedure for 1-ethoxy-2,3-dinitro-4-acetamido-benzene (VI). p-Phenacetin (25 g.) treated during 1 hr. at 15-25.degree. with 125 ml. fuming HNO3, the mixt. poured into 1.5 l. cold H2O, and the product crystd. gave 28.1 g. VI, plates, m. 211-12.degree.. The av. yield of VI from 14 similar runs was 75%. VI (54 g.) in 350 ml. HCONMe2 reduced in the presence of 40 g. 5% Pd-C at room temp./30 lb./sq. in. 1.5 hrs., the mixt. filtered under N into 68.1 g. Na glyoxal bisulfite in 1 l. 70.degree. H2O, refluxed 6 hrs. under N, filtered, the filtrate evapd., and the oil poured into 31. Me2CO gave 21.3 g. I, m. 186.degree.. I (2 g.) and 20 ml. 2NH2SO4 heated 15 min. at 95-8.degree., the soln. cooled, neutralized, and the solid washed and recrystd. gave 1.48 g. II, m. 85-6.degree. (alc.-Me2CO). II appeared to undergo a no. of the usual reactions of aromatic amines. It could be coupled with .beta.-naphthol, 1-phenyl-3-methyl-5-pyrazolone, p-cresol, di-phenylamine, dimethylaniline, and N-ethyl-N-(.beta.-cyano-ethyl)-m-toluidine to form dyes. II (0.5 g.) in 10 ml. alc. stirred 1 hr. at room temp. with excess 14% HCl gave 0.59g. II.HCl, m. 180-90.degree.. p-MeC6H4SO2Cl (0.33 g.) refluxed 0.5 hr. with 0.5 g. II gave 0.48 g. III, m. 132-3.degree. (alc.-Me2CO). IV was obtained in 90.5% yield, m. 223-9.degree..Alc. HCl hydrolysis of IV gave 71% V, yellow, m.

181-2.degree..

L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS
AN 1958:55935 CAPLUS
DN 52:55935
OREF 52:10095e-i,10096a-i,10097a-g
TI Aminoisoquinolines, -cinnolines, and -quinazolines. (A) The basic strengths and ultraviolet absorption spectra. (B) Infrared spectra
AU Osborn, A. R.; Schofield, K.; Short, L. N.
CS Washington Singer Labs., Exeter, UK
SO J. Chem. Soc. (1956) 4191-206
DT Journal
LA Unavailable
IT **16566-20-4**, Quinoxaline, 5-amino- (basicity and spectra of)
RN 16566-20-4 CAPLUS
CN 5-Quinoxalinamine (9CI) (CA INDEX NAME)



AB cf. following abstr. Potentiometric titrations in aq. soln. at 20.degree. with HCl gave the following pKa values. Isoquinolines: unsubstituted (I), 5.40; 3-NH2 (Ia), 5.05; 4-NH2 (Ib), 6.28; 5-NH2 (Ic), 5.59; 6-NH2 (Id), 7.17; 7-NH2 (Ie), 6.20; 8-NH2 (If), 6.06. Cinnolines: unsubstituted (II), 2.29; 3-NH2 (IIa), 3.70; 4-NH2 (IIb), 6.85; 5-NH2 (IIc), 2.70; 6-NH2 (IId), 5.04; 7-NH2 (IIe), 4.85; 8-NH2 (IIf), 3.68. Quinazolines: unsubstituted (III), 3.51; 2-NH2 (IIIa), 4.82; 4-NH2 (IIIb), 5.85; 5-NH2 (IIIc), 3.57; 6-NH2 (IIId), 3.29; 7-NH2 (IIIe), 4.60; 8-NH2 (IIIf), 2.81. In addn. pKa values based on calcns. from ultraviolet extinction curves were detd. for phenanthridine 4.52, its 6-NH2 deriv. 6.88, and 6,7-benzoquinazoline (IV) .apprx. 5.2. Ultraviolet absorption data for the above bases and their cations in buffered aq. solns. and of the methochlorides of I, II, and III in H2O were given. I, II, and III showed the 3 main bands characteristic of electronic transitions parallel to the long, short, and long axes of bicyclic systems, and the effect of the position of the NH2 substitutent could be correlated fairly well with the shifts of the bands noted in the spectra of their NH2 derivs. II in cyclohexane showed an addnl. low-intensity, longer wavelength (390 m.mu.) band of an n .fwdarw. .pi. transition which disappeared in water or acid. The bathochromic shift shown in the spectra of the aminoisoquinolines on conversion to the cations indicated that, as with I, the monocations carry the proton on the ring N. Study of the .DELTA.pKa values (relative to I) showed values below 1 for Ib, Ic, and Ie, in which there is no possibility of addnl. ionic resonance in the cations, and above 1 for the 1-NH2 deriv. of I and Id, for which addnl. forms are possible, and a neg. value for Ia, which is clearly not increased in stability by a possible .omicron.-quinonoid resonance form (see the following abstr. for If). The bathochromic shifts in the spectra of the aminocinnolines on cation formation again indicated that proton attachment is to the ring N. By analogies to the quinoline and isoquinoline series, .DELTA.pKa values indicated that N1 is the predominant basic center in IIb, IIe, and

probably IIc, while N2 is the basic center for IId and IIf (the spectra of If and IIf are similar). From the values of .DELTA.pKa for IIa, the basic center is considered to be N2, although it contrasts strongly with Ia. Cationization of III caused a marked hypsochromic shift in contrast to the more usual slight bathochromic shift for other heterocyclic bases, and some modification of the aromatic system, possibly a 3,4-hydration, is assumed. Ultraviolet studies on cation formation of the aminoquinazolines indicated no hydration for IIIa and IIIb (similar to 2- and 4-aminoquinoline), IIIc, IIIe, and IIIf, while IIId is presumably hydrated. Considering the change on cationization of III and the increased base strength of 3,4-dihydroquinazolines relative to the quinazolines, choice of a basic center by correlation with .DELTA.pKa values is difficult, although N1 seems to be favored for IIIb and definite for IIIe. Quinoxaline and its 6-NH2 deriv. also showed the usual bathochromic shift on cation formation, while the 5-NH2 deriv. seemed to take up the first proton on its NH2 group. Infrared N-H bond stretching frequencies and force constants, indicative of the amt. of interaction of the NH2 group with the ring and the electron density at the ring N, were given for Ia-f, IIa-f, IIIa-f, 2-, 4-, and 5-aminopyrimidines, and 5-aminoquinoline in CCl4, CHCl3, and pyridine (some compds.); the effects of electromeric interaction where possible, the lack of interaction between N1 and a C-5 NH2 group, the effect of 2 ring N atoms adjacent to the NH2 group and of intramolecular H-bonding were noted. 1,3-Dichloroisoquinoline (0.5 g.), 25 cc. MeOH, 0.4 g. KOH, and 3 cc. Raney Ni shaken with H, the MeOH evapd., and the Et2O ext. of the residue treated with picric acid in Et2O gave I picrate, m. 225-6.degree.; 1,3-dibromoisoquinoline (V) behaved similarly. Homophthalimide (5 g.) and 50 cc. PBr3 refluxed 5 hrs., the PBr3 evapd. in vacuo, and the residue treated with alkali gave 3.4 g. V, m. 147-7.5.degree. (MeOH). V (3 g.) was converted to 1.75 g. 3-bromoisoquinoline (VI), m. 63-4.degree. (aq. MeOH). 3-Chloroisoquinoline (8.8 g.), 100 cc. concd. NH4OH, and 1 g. CuSO4 heated 30 hrs. at 140.degree. in an autoclave, made strongly basic, and extd. with CHCl3 gave 5.3 g. Ia, m. 176-7.degree. (C6H6), similarly prepd. from VI. Ib m. 108-9.5.degree. (C6H6-cyclohexane). 5-Nitroisoquinoline (20 g.), 500 cc. MeOH, and 2 g. 5% Pd-C hydrogenated 2 hrs., evapd., and the residue crystd. from CHCl3-petr. ether gave 93% Ic, m. 129.5-30.5.degree. (C6H6-cyclohexane). m-MeOC6H4CHO (35.5 g.), 18 g. MeNO2, 125 cc. HOAc, and 12.5 g. NH4OAc refluxed 2 hrs. and poured into H2O gave 27 g. m-MeOC6H4CH:CHNO2, m. 91-2.degree. (C6H6), which was not reduced satisfactorily. 1,2,3,4-Tetrahydro-6-methoxyisoquinoline (2.42 g.) and 0.8 g. 30% Pd-C heated 0.25 hr. at 180-90.degree. in a stream of N, extd. with Et2O, the 2.1 g. oily product treated with 3 g. picric acid in 10 cc. Me2CO, the 2.9 g. picrate decompd. with aq. LiOH, extd. with Et2O, the 1.03 g. product refluxed 2 hrs. with 25 cc. concd. HBr, evapd. in vacuo, dissolved in 10 cc. H2O, and treated with aq. Na2CO3 gave 0.85 g. 6-hydroxyisoquinoline (VII), m. 220.degree. (decompn.); dehydrogenation with Raney Ni in naphthalene was unsuccessful. Id, m. 211-12.degree. (C6H6), was prepd. from VII. 1,3-Dihydroxy-7-nitroisoquinoline (VIII) (52 g.), m. 291.degree. (decompn.), was prepd. from 56 g. 4-nitrohomophthalic acid in .omicron.-C6H4Cl2. VIII (2 g.) and 20 cc. POCl3 heated 4 hrs. on the steam bath, decompd. with ice, and brought to pH 10 gave 1.18 g. 1,3-dichloro-7-nitroisoquinoline, m. 185.degree. (decompn.) (HOAc), but the reaction was not reproducible. 7-Hydroxyisoquinoline (1.25 g.), 4 cc. NH4SO3 (concd. NH4OH satd. with SO2), and 20 cc. concd. NH4OH 16 hrs. at 140-50.degree. gave 1.1 g. Ie, m. 203-5.degree. (C6H6) after sublimation at 150.degree./0.3 mm. Ic (4.8 g.) in 12 cc. concd. HBr and 13 cc. H2O diazotized at 0.degree. with 2.3 g. NaNO2 in 15 cc. H2O, added to 5.8 g. CuBr in 48 cc. HBr at 75.degree., and let stand 24 hrs. gave 5.1 g.

5-bromoisoquinoline (IX), m. 82-4.degree. (petr. ether). KNO3 (2.4 g.) in 20 cc. concd. H2SO4 added during 5 min. to 4.15 g. IX in 24 cc. concd. H2SO4, the mixt. let stand 1 hr. at room temp., poured on ice, and made alk. with NH4OH gave 5.05 g. 5-bromo-8-nitroisoquinoline (X), m. 139-41.degree. (MeOH). 5-Chloro-8-nitroisoquinoline (2 g.) and 12 g. NH4OAc added to 2 g. 6% Pd-CaCO3 in abs. MeOH (previously shaken with H), hydrogenated 1 hr., the filtered soln. acidified with concd. HCl, the MeOH evapd. in vacuo, the residue in H2O made alk. with satd. Na2CO3, and extd. with CHCl3 gave 1.02 g. If, m. 171-2.degree. (EtOAc); use of NaOAc in the reduction gave lower yields of If while reduction with Pd-C in MeOH in the presence of NaOAc gave 8-amino-5-chloroisoquinoline, from which the Cl was not removed on Raney Ni hydrogenation in alk. soln.; hydrogenation of X in MeOH over Pd-CaCO3 gave colored intermediate products, while reduction of X in the presence of KOH gave a small yield of If. 2-Chloroquinazoline (0.5 g.) added slowly to 0.4 g. KOH in 5 g. PhOH, the mixt. heated 3 hrs. at 70.degree., and made alk. gave 0.58 g. 2-phenoxyquinazoline (XI), m. 124-6.degree. (petr. ether). XI (0.5 g.) and 5 g. NH4OAc heated 2 hrs. at 170-80.degree. and treated with H2O and 2N NaOH gave 0.35 g. IIIa, m. 200.degree. (EtOH). IIIb m. 271-2.degree. (EtOH). 6,2-O2N(H2N)C6H3CO2H (14.84 g.) and 29.4 cc. HCONH2 4.5 hrs. at 155-60.degree. gave 12.2 g. 4-hydroxy-5-nitroquinazoline (XII), m. 252-6.degree. (H2O). XII (7 g.) and POCl3 gave 5.17 g. 4-chloro-5-nitroquinazoline (XIII), m. 142.degree. after sublimation at 140.degree./0.5 mm. Resublimed XIII (1 g.) in 150 cc. dry MeOCH2CH2OH and 0.5 g. 6% Pd-CaCO3 hydrogenated 0.5 hr., evapd., oxidized with K3Fe(CN)6, and the product chromatographed gave 0.265 g. IIIc, m. 195-6.5.degree. (C6H6) after sublimation at 160.degree./1 mm. IIId, m. 213-14.degree. (C6H6), IIIe, m. 190-1.degree. (C6H6) after sublimation at 160.degree./0.5 mm., and IIIf, m. 150-1.degree. after sublimation at 120.degree./0.5 mm., were prepd. similarly by reduction at atm. pressure with 6% Pd-C. 1-Chloro-7-methoxyphthalazine (XIV) (7.4 g.), m. 142.degree. (decompn.), was obtained by refluxing 8.8 g. 1-OH compd. 0.5 hr. with 40 cc. POCl3. XIV (0.5 g.), 0.2 g. red P, and 5 cc. HI refluxed 1 hr., dild. with 5 cc. H2O, evapd. in vacuo, and the residue in 5 cc. H2O adjusted to pH 7 with NH4OH gave 0.3 g. 6-hydroxyphthalazine-0.5H2O, m. 300.degree. (decompn.) (H2O), which was not converted successfully to the 6-NH2 compd. XIV refluxed with HBr gave 4,6-dihydroxyphthalazine, m. 310.degree. (decompn.) (H2O). 3,2-H2NC10H6CO2H (10 g.) was converted to 8.5 g. 4-hydroxy-6,7-benzoquinazoline (XV), m. 278.degree. (H2O). XV (1.3 g.) and 20 cc. POCl3 refluxed 2 hrs. gave 0.98 g. 4-chloro-6,7-benzoquinazoline (XVI), m. 176-8.degree. after sublimation at 160.degree./0.1 mm. XVI (0.4 g.) in 50 cc. MeOCH2CH2OH hydrogenated 1.5 hrs. over 0.5 g. 8% Pd-CaCO3 and the product in H2O oxidized with 1.4 g. K3Fe(CN)6 gave 0.19 g. IV, m. 163-5.degree. (cyclohexane) after sublimation. XVI (0.23 g.) and 25 cc. satd. NH3-MeOH refluxed 2 hrs. gave 4-amino-6,7-benzoquinazoline, m. 365.degree. (decompn.) (EtOH) after repeated sublimation. XVI (2.1 g.) in 100 cc. warm C6H6 added to 2 equivs. NaCH(CO2Et)2 in 100 cc. C6H6, refluxed 3 hrs., let stand overnight, poured into H2O, the org. layer evapd., and the residue crystd. from EtOH gave 2.29 g. di-Et 6,7-benzoquinazol-4-ylmalonate (XVII), m. 172-5.degree.. XVII (1.5 g.), 0.6 g. KOH, and 60 cc. MeOH refluxed 3 hrs. gave 0.58 g. 6,7-benzoquinazol-4-ylacetate, m. 207-9.degree. (MeOH), hydrolyzed with boiling aq. NaOH to traces of 4-methyl-6,7-benzoquinazoline-1.5H2O, m. 124-6.degree. (petr. ether). I (5 g.), 10 cc. MeI, and MeOH refluxed 2 hrs. gave I methiodide, m. 160-1.5.degree. (EtOH), which was shaken with 50 cc. H2O and excess freshly pptd. AgCl for 12 hrs., filtered, the filtrate evapd., and I methochloride crystd. under anhyd. conditions from EtOH-Et2O. Quinoline methochloride, the very deliquescent II

methochloride-0.5H2O, and 4-methylcinnoline methochloride-H2O were prepd. similarly.

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NEWS 17	Dec 17	TOXCENTER enhanced with additional content
NEWS 18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20	Feb 13	CANCERLIT is no longer being updated
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NEWS 24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 25	Feb 26	PCTFULL now contains images
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NEWS 29	Mar 24	PATDPAFULL now available on STN
NEWS 30	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 31	Apr 11	Display formats in DGENE enhanced
NEWS 32	Apr 14	MEDLINE Reload
NEWS 33	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 34	Apr 21	Indexing from 1947 to 1956 being added to records in CA/CAPLUS
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STRUCTURE FILE UPDATES:    2 MAY 2003  HIGHEST RN 509953-09-7
DICTIONARY FILE UPDATES:   2 MAY 2003  HIGHEST RN 509953-09-7

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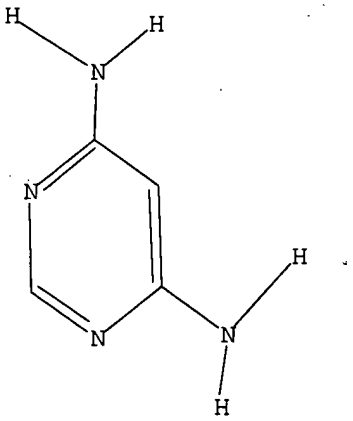
L1 STR



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SAMPLE SEARCH INITIATED 10:52:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 630 TO ITERATE

100.0% PROCESSED 630 ITERATIONS 50 ANSWERS
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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 11095 TO 14105
PROJECTED ANSWERS: 1384 TO 2576

L2 50 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:52:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 12545 TO ITERATE

100.0% PROCESSED 12545 ITERATIONS 1870 ANSWERS

SEARCH TIME: 00.00.01

L3 1870 SEA SSS FUL L1

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FILE COVERS 1907 - 3 May 2003 VOL 138 ISS 19
FILE LAST UPDATED: 2 May 2003 (20030502/ED)

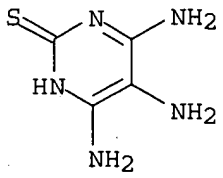
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1498 L3

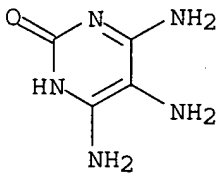
=> s l4 and quinoxaline
L5 10 L4 AND QUINOXALINE

=> d l5 fbib hitstr abs total

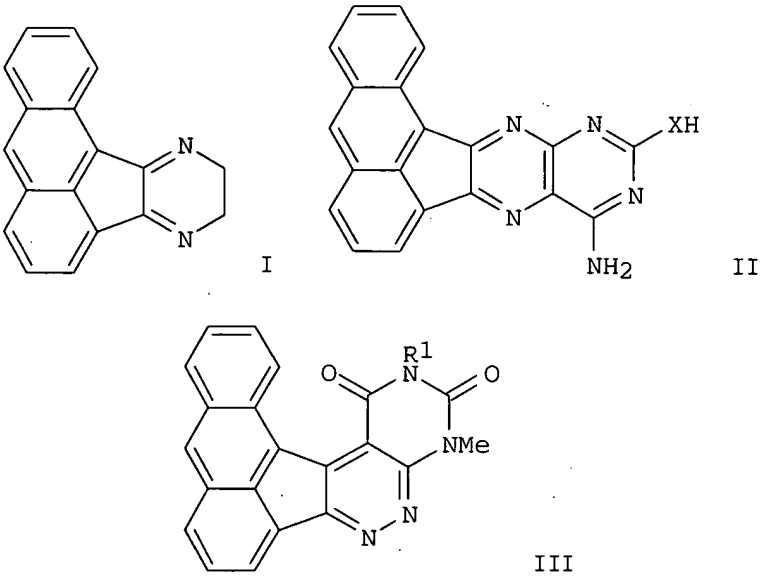
L5 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 2002:224567 CAPLUS
DN 137:109252
TI On condensation reactions of aceanthrenequinone: novel heterocycles
AU Amer, Atef M.; El-Mobayed, Medhat; Ateya, Abdel M.; Muhdi, Tarek S.
CS Chemistry Department, Faculty of Science, Zagazig University, Zagazig, Egypt
SO Monatshefte fuer Chemie (2002), 133(1), 79-88
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer-Verlag Wien
DT Journal
LA English
OS CASREACT 137:109252
IT **1073-99-0**, 4,5,6-Triamino-2-pyrimidinethiol **22715-34-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(heterocycle prepn. by condensation reactions of aceanthrenequinone)
RN 1073-99-0 CAPLUS
CN 2(1H)-Pyrimidinethione, 4,5,6-triamino- (9CI) (CA INDEX NAME)



RN 22715-34-0 CAPLUS
CN 2(1H)-Pyrimidinone, 4,5,6-triamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



GI



I II III

AB It was found that aceanthrenequinone can be condensed with ethylenediamine, 1,2-diaminobenzene, 4-nitro-1,2-diaminobenzene, 1,2-diaminoanthrenequinone, and 4,5,6-triaminopyrimidine derivs. to give aceanthryleno[1,2-b]pyrazine (I) and aceanthryleno[1,2-g]pteridine derivs. (II; X = O, S). Condensation of aceanthrenequinone with 2-aminoguanidine, semicarbazide, and thiosemicarbazide yielded aceanthryleno[1,2-e]triazines; condensation with 6-hydrazinopyrimidine derivs. gave 3,4-aceanthrylenopyrimido[4,5-c]pyridazines (III; R1 = Me, H). Reaction

of aceanthrenequinone with 2-cyanoethanoic acid hydrazide afforded 10,11-dihydro-10-oxoaceanthryleno[1,2-c]pyridazine-9-carbonitrile. Treatment of aceanthrenequinone with malononitrile and hydrazine hydrate resulted in 10-aminoaceanthryleno[1,2-c]pyridazine-9-carbonitrile. The antibacterial effects of the prepd. compds. were tested. Three of the compds. were tested against 60 cancer types.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 2001:923229 CAPLUS
DN 136:58496
TI Hair dyeing compositions containing **quinoxaline** derivatives
IN Gross, Wibke; Hoeffkes, Horst; Martin, Hans-Dieter; Moeller, Hinrich; Oberkobusch, Doris
PA Henkel K.-G.a.A., Germany
SO Ger. Offen., 22 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10029929	A1	20011220	DE 2000-10029929	20000617
WO 2001097754	A2	20011227	WO 2001-EP6544	20010609
WO 2001097754	A3	20020523		
W: AU, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
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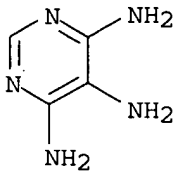
EP 1292271	A2	20030319	EP 2001-957836	20010609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
			DE 2000-10029929A	20000617
			WO 2001-EP6544 W	20010609

OS MARPAT 136:58496
IT **118-70-7**, 4,5,6-Triaminopyrimidine **1004-74-6**, 2,4,5,6-Tetraaminopyrimidine **5392-28-9 22715-34-0**, 2-Hydroxy-4,5,6-Triaminopyrimidine **62496-02-0**, 2-Methylamino-4,5,6-triaminopyrimidine
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(hair dyeing compns. contg. **quinoxaline** derivs.)
RN 118-70-7 CAPLUS
CN 4,5,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



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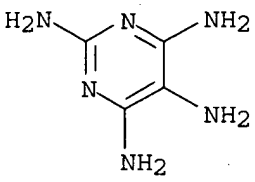
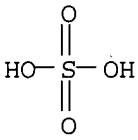
CN Pyrimidinetetramine (9CI) (CA INDEX NAME)



RN 5392-28-9 CAPLUS
CN Pyrimidinetetramine, sulfate (1:1) (9CI) (CA INDEX NAME)

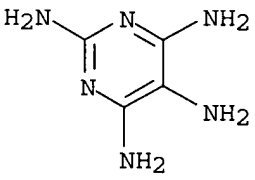
CM 1

CRN 7664-93-9
CMF H2 O4 S

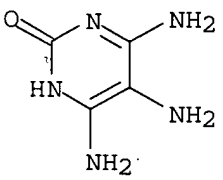


CM 2

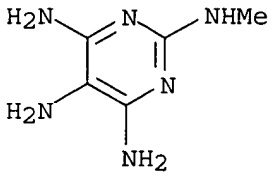
CRN 1004-74-6
CMF C4 H8 N6



RN 22715-34-0 CAPLUS
CN 2(1H)-Pyrimidinone, 4,5,6-triamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 62496-02-0 CAPLUS
CN Pyrimidinetetramine, N2-methyl- (9CI) (CA INDEX NAME)



AB Hair dye compns. contain at least one **quinoxaline** deriv. contg. e.g., C1-4 alkenyl, hydroxyalkyl, carboxyalkyl groups, and halo groups. Thus, 1,1,3-trimethylcyclo-2-penten[1,2-b]quinozaline-2-carboxaldehyde (I) was prepd. in a seies of steps and formulated into a hair dye formulation contg. I 4.4, Natrosol 250HR 2.0 and water to 100.0 g.

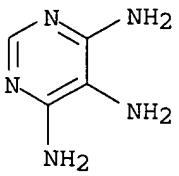
L5 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 2001:45037 CAPLUS
DN 134:120569
TI Hair dyeing preparations containing heterocyclic aldehydes or ketones
IN Moeller, Hinrich; Oberkobusch, Doris; Hoeffkes, Horst
PA Henkel K.-G.a.a., Germany
SO Ger. Offen., 12 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19933187	A1	20010118	DE 1999-19933187	19990715
WO 2001005359	A2	20010125	WO 2000-EP6399	20000706
WO 2001005359	A3	20010426		

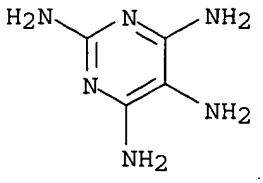
W: AU, JP, US
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

DE 1999-19933187A 19990715

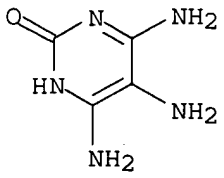
OS MARPAT 134:120569
IT **118-70-7**, 4,5,6-Triaminopyrimidine **1004-74-6**, 2,4,5,6-Tetraaminopyrimidine **22715-34-0**, 2-Hydroxy-4,5,6-triaminopyrimidine **62496-02-0**, 2-Methylamino-4,5,6-triaminopyrimidine
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(hair dyeing prepns. contg. heterocyclic aldehydes or ketones)
RN 118-70-7 CAPLUS
CN 4,5,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



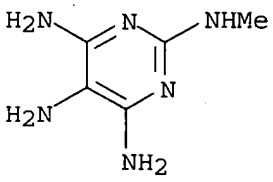
RN 1004-74-6 CAPLUS
CN Pyrimidinetetramine (9CI) (CA INDEX NAME)



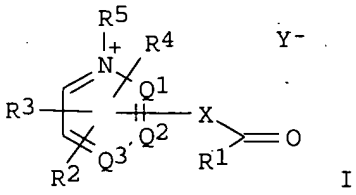
RN 22715-34-0 CAPLUS
CN 2(1H)-Pyrimidinone, 4,5,6-triamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 62496-02-0 CAPLUS
CN Pyrimidinetetramine, N2-methyl- (9CI) (CA INDEX NAME)



GI



I

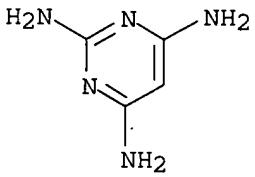
AB The invention concerns compns. for dyeing keratin fibers, esp. hair, that contain at least one heterocyclic aldehyde or ketone of the formula (I) and a compd. from the group of arom. amines, hydroxyls,inculuding heterocycles, and compds. with active CH groups. In I R1 = H, C1-C4 alkyl, aryl, heteroaryl; R2, R3, R4 = H, C1-C4 alkyl, hydroxyalkyl, carboxyalkyl, sulfoalkyl, aryl, aralkyl, hetoroaryl; Q1, Q2, Q3 = combination of two C and one N, the N can be quaternized; X = vinylene or vinylene deriv.; Y = halide, benzene sulfonate, p-toluene sulfonate, methane sulfonate, tetrachlorozincate, nitrogen oxide, oxide. Thus 2-formyl-1-methylquinoxalinium-trifluoromethanesulfonate was synthesized from **quinoxaline**-2-carboxaldehyde and trifluoromethanesulfonic acid Me ester. The product was used in hair dyeing compns.; depending on the selected other dye(s), different colors were obtained; e.g the

combination with 2-methyl-3-amino-6-methoxypyridine dihydrochloride resulted redish brown hair color.

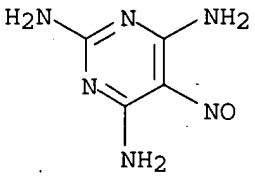
L5 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 1996:333008 CAPLUS
DN 125:127644
TI Method for obtaining improved image contrast in migration imaging members
IN Limburg, William W.; Mammino, Joseph; Liebermann, George; Griffiths, Clifford H.; Shahin, Michael M.; Malhotra, Shadi L.; Chen, Liqin; Perron, Marie-Eve
PA Xerox Corp., USA
SO U.S., 147 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5514505	A	19960507	US 1995-441360	19950515
	CA 2169980	AA	19961116	CA 1996-2169980	19960221
	CA 2169980	C	20010424		
				US 1995-441360 A	19950515
	JP 08314240	A2	19961129	JP 1996-113456	19960508
				US 1995-441360 A	19950515
	EP 743573	A2	19961120	EP 1996-303359	19960514
	EP 743573	A3	19970305		
	EP 743573	B1	20000906		
	R: DE, FR, GB				
				US 1995-441360 A	19950515

OS MARPAT 125:127644
IT **1004-38-2**, 2,4,6-Triaminopyrimidine **1006-23-1**, 5-Nitroso-2,4,6-triaminopyrimidine **49647-58-7**, 2,4,5,6-Tetraaminopyrimidine sulfate **49721-45-1** **116295-66-0 120407-07-0**
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(transparentizing agent for electrophotog. migration imaging members)
RN 1004-38-2 CAPLUS
CN 2,4,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



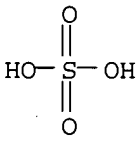
RN 1006-23-1 CAPLUS
CN 2,4,6-Pyrimidinetriamine, 5-nitroso- (9CI) (CA INDEX NAME)



RN 49647-58-7 CAPLUS
CN Pyrimidinetetramine, sulfate (9CI) (CA INDEX NAME)

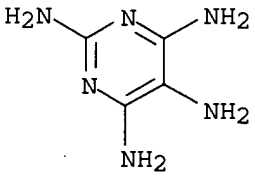
CM 1

CRN 7664-93-9
CMF H2 O4 S



CM 2

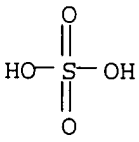
CRN 1004-74-6
CMF C4 H8 N6



RN 49721-45-1 CAPLUS
CN 4,5,6-Pyrimidinetriamine, sulfate (1:1) (9CI) (CA INDEX NAME)

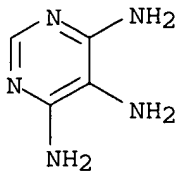
CM 1

CRN 7664-93-9
CMF H2 O4 S



CM 2

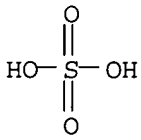
CRN 118-70-7
CMF C4 H7 N5



RN 116295-66-0 CAPLUS
CN 2(1H)-Pyrimidinethione, 4,5,6-triamino-, sulfate (1:1) (9CI) (CA INDEX NAME)

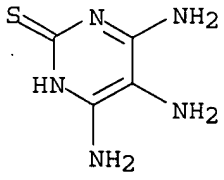
CM 1

CRN 7664-93-9
CMF H2 O4 S

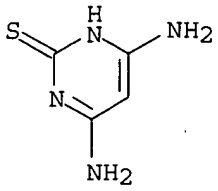


CM 2

CRN 1073-99-0
CMF C4 H7 N5 S



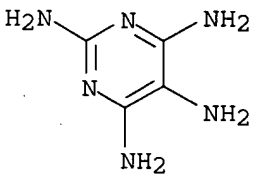
RN 120407-07-0 CAPLUS
CN 2(1H)-Pyrimidinethione, 4,6-diamino-, hydrate (2:1) (9CI) (CA INDEX NAME)



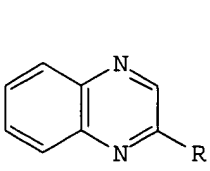
1/2 H_2O

AB Disclosed is a process which comprises (a) providing a migration imaging member comprising (1) a substrate and (2) a softenable layer comprising a softenable material and a photosensitive migration marking material present in the softenable layer as a monolayer of particles situated at or near the surface of the softenable layer spaced from the substrate, (b) uniformly charging the imaging member, (c) imagewise exposing the charged imaging member to activating radiation at a wavelength to which the migration marking material is sensitive, (d) causing the softenable material to soften and enabling a first portion of the migration marking material to migrate through the softenable material toward the substrate in an imagewise pattern while a second portion of the migration marking material remains substantially unmigrated within the softenable layer, and (e) contacting the second portion of the migration marking material with a transparentizing agent which transparentizes the migration marking material.

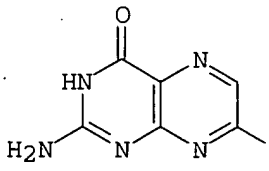
L5 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 1984:571208 CAPLUS
DN 101:171208
TI 1-Halo-1-(acylamino)-2-alkanones as synthons for the preparation of **quinoxalines** and pteridines
AU Zav'yalov, S. I.; Ezhova, G. I.; Budkova, T. K.
CS Inst. Org. Khim. im. Zelinskogo, Moscow, USSR
SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1984), (7), 1590-3
CODEN: IASKA6; ISSN: 0002-3353
DT Journal
LA Russian
OS CASREACT 101:171208
IT **1004-74-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with (acylamino)haloalkanones)
RN 1004-74-6 CAPLUS
CN Pyrimidinetetramine (9CI) (CA INDEX NAME)



GI



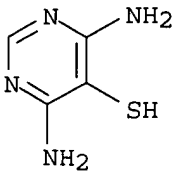
I



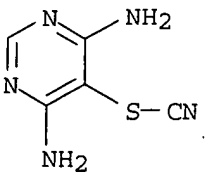
II

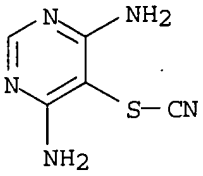
AB Alkylquinoxalines I (R = Me, Et, Pr) and 7-alkylpteridines II (R = Me, Et) were prepd. in 52-70% and 68-80% yields, resp., by cyclocondensation of RCOCHXNHCOR1 (X = Cl, Br; R1 = Me, Ph) with o-phenylenediamine or 2,5,6-triamino-2(1H)-pyrimidinone (III). Treating AcNHCHBrCOMe with N2H4.cntdot.H2O gave 29% HC(:NHNH2)C(:NHNH2)Me which was cyclocondensed with III to give 84% 6-methylpteridine and 16% II (R = Me).

L5 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 1981:208808 CAPLUS
DN 94:208808
TI Studies in the heterocyclic series. XVIII. Utilization of 4-aminopyrimidine chemistry in 1,4,7,9-tetraazabenzo[b]phenothiazine synthesis
AU Okafor, Charles O.
CS Dep. Chem., Univ. Nigeria, Nigeria, Nigeria
SO Journal of Heterocyclic Chemistry (1980), 17(7), 1587-92
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
IT **77709-01-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization with dichlorophenoxalines)
RN 77709-01-4 CAPLUS
CN 5-Pyrimidinethiol, 4,6-diamino- (9CI) (CA INDEX NAME)

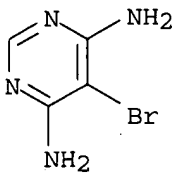


IT **30161-88-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)
RN 30161-88-7 CAPLUS
CN Thiocyanic acid, 4,6-diamino-5-pyrimidinyl ester (9CI) (CA INDEX NAME)





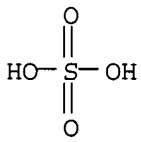
IT **58023-98-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with thiocyanate)
RN 58023-98-6 CAPLUS
CN 4,6-Pyrimidinediamine, 5-bromo- (9CI) (CA INDEX NAME)



IT **77709-02-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sodium thiocyanate)
RN 77709-02-5 CAPLUS
CN 4,6-Pyrimidinediamine, sulfate (2:1) (9CI) (CA INDEX NAME)

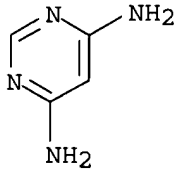
CM 1

CRN 7664-93-9
CMF H2 O4 S



CM 2

CRN 2434-56-2
CMF C4 H6 N4



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NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Jun 03	New e-mail delivery for search results now available
NEWS 4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 7	Sep 03	JAPIO has been reloaded and enhanced
NEWS 8	Sep 16	Experimental properties added to the REGISTRY file
NEWS 9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11	Oct 24	BEILSTEIN adds new search fields
NEWS 12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13	Nov 18	DKILIT has been renamed APOLLIT
NEWS 14	Nov 25	More calculated properties added to REGISTRY
NEWS 15	Dec 04	CSA files on STN
NEWS 16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17	Dec 17	TOXCENTER enhanced with additional content
NEWS 18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20	Feb 13	CANCERLIT is no longer being updated
NEWS 21	Feb 24	METADEX enhancements
NEWS 22	Feb 24	PCTGEN now available on STN
NEWS 23	Feb 24	TEMA now available on STN
NEWS 24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 25	Feb 26	PCTFULL now contains images
NEWS 26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27	Mar 19	APOLLIT offering free connect time in April 2003
NEWS 28	Mar 20	EVENTLINE will be removed from STN
NEWS 29	Mar 24	PATDPAFULL now available on STN
NEWS 30	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 31	Apr 11	Display formats in DGENE enhanced
NEWS 32	Apr 14	MEDLINE Reload
NEWS 33	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 34	Apr 21	Indexing from 1947 to 1956 being added to records in CA/CAPLUS
NEWS 35	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 36	Apr 28	RDISCLOSURE now available on STN

NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003

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 NEWS WWW      CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 11:00:30 ON 03 MAY 2003

=> le reg
LE IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                0.21       0.21

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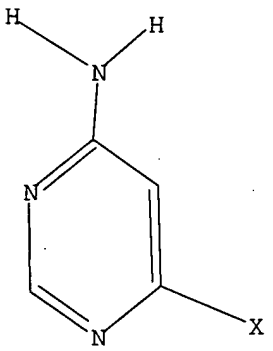
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10077150.5

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 11:01:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 512 TO ITERATE

100.0% PROCESSED 512 ITERATIONS 38 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8883 TO 11597
PROJECTED ANSWERS: 391 TO 1129

L2 38 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 11:01:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 10484 TO ITERATE

100.0% PROCESSED 10484 ITERATIONS 762 ANSWERS
SEARCH TIME: 00.00.01

L3 762 SEA SSS FUL L1

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=> file caplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       148.15     148.36

FILE 'CAPLUS' ENTERED AT 11:01:13 ON 03 MAY 2003
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FILE COVERS 1907 - 3 May 2003  VOL 138 ISS 19
FILE LAST UPDATED: 2 May 2003  (20030502/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l3
L4          742 L3

=> s l4 and qunopxaline
L5            0 L4 AND QUNOPXALINE

=> s l4 and quinoxaline
L6            2 L4 AND QUINOXALINE

=> d l6 fbib hitstr abs total

L6   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2003 ACS
AN   1996:333008  CAPLUS
DN   125:127644
TI   Method for obtaining improved image contrast in migration imaging members
IN   Limburg, William W.; Mammino, Joseph; Liebermann, George; Griffiths,
     Clifford H.; Shahin, Michael M.; Malhotra, Shadi L.; Chen, Liqin; Perron,
     Marie-Eve
PA   Xerox Corp., USA
SO   U.S., 147 pp.
     CODEN: USXXAM
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
     ----------------  ----  --------      ---------------  --------
PI   US 5514505         A    19960507      US 1995-441360   19950515
     CA 2169980         AA   19961116      CA 1996-2169980  19960221
     CA 2169980         C    20010424
                                           US 1995-441360 A 19950515
```

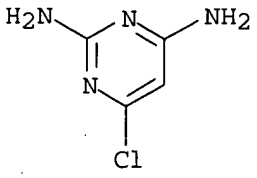
JP 08314240	A2	19961129	JP 1996-113456	19960508
			US 1995-441360 A	19950515
EP 743573	A2	19961120	EP 1996-303359	19960514
EP 743573	A3	19970305		
EP 743573	B1	20000906		
R: DE, FR, GB				
			US 1995-441360 A	19950515

OS MARPAT 125:127644

IT **156-83-2**, 2,6-Diamino-4-chloropyrimidine
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(transparentizing agent for electrophotog. migration imaging members)

RN 156-83-2 CAPLUS

CN 2,4-Pyrimidinediamine, 6-chloro- (9CI) (CA INDEX NAME)



AB Disclosed is a process which comprises (a) providing a migration imaging member comprising (1) a substrate and (2) a softenable layer comprising a softenable material and a photosensitive migration marking material present in the softenable layer as a monolayer of particles situated at or near the surface of the softenable layer spaced from the substrate, (b) uniformly charging the imaging member, (c) imagewise exposing the charged imaging member to activating radiation at a wavelength to which the migration marking material is sensitive, (d) causing the softenable material to soften and enabling a first portion of the migration marking material to migrate through the softenable material toward the substrate in an imagewise pattern while a second portion of the migration marking material remains substantially unmigrated within the softenable layer, and (e) contacting the second portion of the migration marking material with a transparentizing agent which transparentizes the migration marking material.

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

AN 1963:33381 CAPLUS

DN 58:33381

OREF 58:5675f-h,5676a-b

TI v-Triazolo[4,5-d]pyrimidines. II. O-Substituted derivatives of 8-azaguanine and 8-azahypoxanthine

AU Fulmer Shealy, Y.; Clayton, Joe D.; Allen O'Dell, C.; Montgomery, John A.

CS Southern Res. Inst., Birmingham, AL

SO J. Org. Chem. (1962), 27, 4518-23
CODEN: JOCEAH; ISSN: 0022-3263

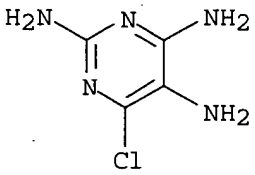
DT Journal

LA Unavailable

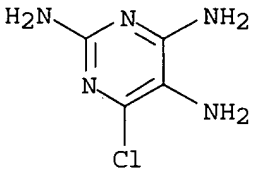
IT **1194-78-1**, Pyrimidine, 2,4,5-triamino-6-chloro- **89303-96-8**, Pyrimidine, 2,4,5-triamino-6-chloro-, hydrochloride
(prepn. of)

RN 1194-78-1 CAPLUS

CN 2,4,5-Pyrimidinetriamine, 6-chloro- (9CI) (CA INDEX NAME)



RN 89303-96-8 CAPLUS
CN Pyrimidine, 2,4,5-triamino-6-chloro-, hydrochloride (7CI) (CA INDEX NAME)

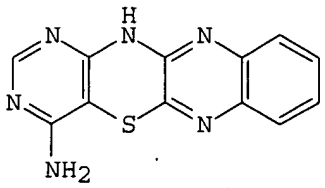


●x HCl

GI For diagram(s), see printed CA Issue.

AB cf. CA 56, 14277g. 5-Amino-7-chloro-v-triazolo[4,5-d]pyrimidine (I) was prepd. from 2,4,5-triamino-6-chloropyrimidine and isoamyl nitrite. 7-Chloro-v-triazolo[4,5-d]pyrimidine was obtained in dioxane soln. by the same method. These compds., useful intermediates for the preparation of a variety of 7-substituted v-triazolo[4,5-d]pyrimidines, were employed in the synthesis of 7-alkoxy- and 7-aryloxy-v-triazolo-[4,5-d] pyrimidines. Preparation and some reactions of 3-bromo-4,5-diaminopyridine. Jan Sylwester Wieezorek and Tadeusz Talik (Politechnika, Wroclaw, Poland). Roczniki Chem. 36, 967-70(1962). I (R = Br, R1 = NH2, R2 = R3 = H) (15 g.) in 75 ml. concd. H2SO4 treated with 30 ml. concd. HNO3 (d. 1.52) at 0 to -10.degree. gave 84.6% I (R = Br, R1 = NHNO2, R2 = R3 = H) (II), m. 203.degree. (decompn.). II (15 g.), when heated with 90 ml. H2SO4 on a steam bath, poured into 500 g. ice and alkalized, gave 14.6 g. I (R = Br, R1 = NH2, R2 = NO2, R3 = H) (III), m. 179-80.degree.. III (3 g.) in 90 ml. glacial AcOH was reduced with 9 g. powd. Fe, heated 1 hr. on steam bath, excess AcOH evapd. under reduced pressure, the residue alkalized, and extd. continuously with Et2O to give 1.8 g. I (R = Br, R1 = R2 = NH2, R3 = H) (IV), m. 140-1.degree.; picrate m. 220-1.degree.. Redn. of III with SnCl2 gave C5H5N3ClBr (m. 206-8.degree., 63.6%), probably I (R = Br, R1 = R2 = NH2, R3 = Cl). IV reacted with phenanthrenequinone to yield 9,10-phenanthro-5,6-(3-bromo-4,5-pyrido)pyrazine, m. 224-6.degree., with 100% HCO2H, 4,5-(3-bromo-4,5-pyrido)imidazole, m. 292-4.degree., and with Bz2, V, m. 198-200.degree..

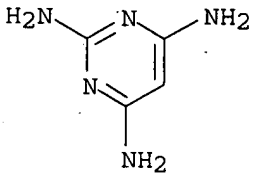
GI



I

AB Tetraazabenzophenothiazine derivs., e.g. I, were prepd. from 4-aminopyrimidines. This new heterocyclic ring was obtained by converting a 4-aminopyrimidine to the corresponding 5-thiocyanato deriv. followed by hydrolysis and subsequent treatment with 2,3-dichloroquinoxaline. Several derivs. were obtained by using suitable substituted starting materials. Nitration with HNO3-H2SO4 gave the corresponding 13-nitro derivs.

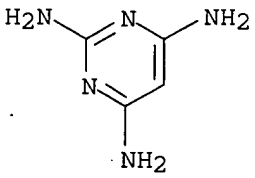
L5 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 1964:64994 CAPLUS
DN 60:64994
OREF 60:11441f-g
TI X-ray powder diffraction patterns of solid hydrocarbons, derivatives of hydrocarbons, phenols, and organic bases
AU Hofer, L. J. E.; Peebles, W. C.; Bean, E. H.
CS U.S. Bur. of Mines, Washington, DC
SO U.S., Bur. Mines, Bull. (1963), No. 613, 59 pp.
DT Journal
LA Unavailable
IT **1004-38-2**, Pyrimidine, 2,4,6-triamino-
(x-ray diffraction pattern for)
RN 1004-38-2 CAPLUS
CN 2,4,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



AB Included are compds. of interest in research involving fuels, coal tar dyes, plastics, pharmaceutical, agricultural chemicals, carcinogens, air pollutants, and other public health problems. X-ray powder diffraction patterns (178) are presented of aromatic hydrocarbons, 2,4,7-trinitro-9-fluorenone derivs. of aromatic hydrocarbons, phenols, and org. bases for pos. identification of solid org. compds.

L5 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 1962:21276 CAPLUS
DN 56:21276
OREF 56:4039d-g
TI Screening of antineoplastic agents with Neurospora crassa
AU Fuerst, Robert

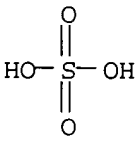
CS Texas Woman's Univ., Denton
SO Develop. Ind. Microbiol. (1960), 1, 101-7
DT Journal
LA Unavailable
IT **1004-38-2**, Pyrimidine, 2,4,6-triamino- **49647-58-7**, Pyrimidine, 2,4,5,6-tetraamino-, sulfate
(effect on 4-aminopyrazolo[3,4-d]pyrimidine deriv. inhibition of Neurospora crassa)
RN 1004-38-2 CAPLUS
CN 2,4,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



RN 49647-58-7 CAPLUS
CN Pyrimidinetetramine, sulfate (9CI) (CA INDEX NAME)

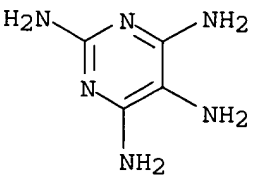
CM 1

CRN 7664-93-9
CMF H2 O4 S



CM 2

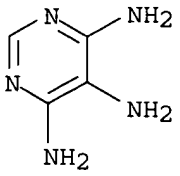
CRN 1004-74-6
CMF C4 H8 N6



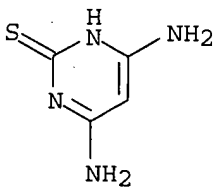
AB Compds. of the 4-aminopyrazolo[3,4-d]pyrimidine (4-APP) compds. and derivs. of 4-APP were tested as antineoplastic agents with N. crassa in liquid culture. Two recent derivs. of 4-APP, 1-methyl-4-octylaminopyrazolo[3,4-d]pyrimidine and 4-heptylamino-1-methylpyrazolo[3,4-d]pyrimidine were more inhibitory to Neurospora than 4-APP itself. **Quinoxalines** a@d isonitrosomalonitriles were also studied; 2-amino-6-purinethiol and many of its derivs. gave little or no

inhibition. Of the most important inhibitors studied, 6-diazo-5-oxonorleucine (DON) gave the best inhibition in lowest doses. Testing DON by the Neurospora agar plate method gave results analogous to the liquid culture method. Thiophene compds. showed definite inhibition but inject/on into C57 black mice resulted in some paralysis and death; 4-(2-thienyl)butanoie acid was the best inhibitor; 2-heptylthiophene and 2-(2-methyl- propyl)thiophene also inhibited well. Aminopterin and 4-APP tested together resulted in 4-APP acting as a relief agent and did not reverse aminopterin inhibition. Inhibition by 4-APP was not affected by 6-methyl-2-thiouracil or purine. 2-Aminopurine and 2,4,5-triamino-6hydroxypyrimidine sulfate increased 4-APP inhibition. DON with azaserine, 4-APP with azaserine, and DON with 8-azaadenine resulted in enhanced inhibition. 8-Azaadenine with azaserine did not affect inhibition. Neurospora as a tool for new chem. antineoplastic agents is important but not more important than the use of other microorganisms or tissue culture techniques or animal-tumor expts.

L5 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 1957:11927 CAPLUS
DN 51:11927
OREF 51:2455d-h
TI Legal's color reaction
AU Tanabe, Yoshihisa; Kamiya, Akiko
CS Kanazawa Univ.
SO Ann. Rept. Fac. Pharm., Kanazawa Univ. (1956), 6, 12-15
DT Journal
LA Unavailable
IT **118-70-7**, Pyrimidine, 4,5,6-triamino- **1004-39-3**, 2-Pyrimidinethiol, 4,6-diamino- **1073-99-0**, 2-Pyrimidinethiol, 4,5,6-triamino- **2434-56-2**, Pyrimidine, 4,6-diamino- **5122-36-1**, Formamide, N-(4,6-diamino-5-pyrimidinyl)- (detection of)
RN 118-70-7 CAPLUS
CN 4,5,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)

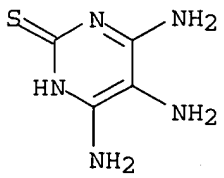


RN 1004-39-3 CAPLUS
CN 2(1H)-Pyrimidinethione, 4,6-diamino- (7CI, 9CI) (CA INDEX NAME)

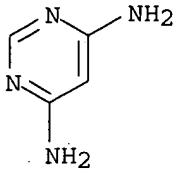


RN 1073-99-0 CAPLUS

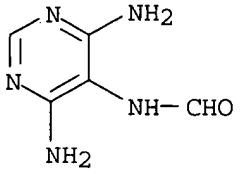
CN 2(1H)-Pyrimidinethione, 4,5,6-triamino- (9CI) (CA INDEX NAME)



RN 2434-56-2 CAPLUS
CN 4,6-Pyrimidinediamine (9CI) (CA INDEX NAME)



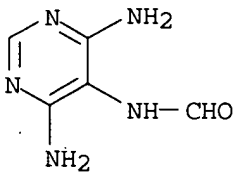
RN 5122-36-1 CAPLUS
CN Formamide, N-(4,6-diamino-5-pyrimidinyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



AB Legal's color reaction was carried out with barbituric acid, purine, pyrimidine, imidazole, etc., and their derivs. The compd., color in basic medium, and color in acidic medium are given (*signifies the color when warmed): barbituric acid, yellow, light yellow (bluish green*); 5-nitrobarbituric acid, orange, light yellow (bluish green*); 5-aminobarbituric acid, yellow, green; 5-isonitrosobarbituric acid, red, deep blue; 5-hydroxybarbituric acid, yellowish brown, orange to red; 5,5-diethylbarbituric acid, yellow, light yellow; 5-ethyl-5-phenylbarbituric acid, yellow, light yellow; 5-ethyl-5-isoamylbarbituric acid, yellow, light yellow; 5-ethyl-5-(1-methylbutyl)barbituric acid, yellow, light yellow; 1-methyl-5-ethyl-5-phenylbarbituric acid, yellow, light yellow; 1,5-dimethyl-5-cyclohexenylbarbituric acid, yellow, light yellow; 5-ethyl-5-cyclohexenylbarbituric acid, yellow, light yellow; thiobarbituric acid, yellow, dark green to dark blue; 5-nitrothiobarbituric acid, orange-yellow, light brown; 5-aminothiobarbituric acid, reddish brown, dark-bluish green; urea, yellow, light yellow; thiourea, yellow, blue to dark blue; methionine, yellow, reddish orange*; theophylline, yellow, light yellow; theobromine, yellow, light yellow; xanthine, yellow, light yellow; caffeine, yellow, light yellow; uric acid, yellow, bluish green*; 4,6-diaminopyrimidine-2-thiol, dark yellow, blue; 4,5,6-triaminopyrimidine-2-thiol, dark yellow, bluish green; 4,6-diaminopyrimidine, yellow, light yellow; 4,5,6-

triaminopyrimidine, yellow, light-reddish orange to reddish orange; 5-formylamino-4,6-diaminopyrimidine, yellow, light yellow; benzimidazole, yellowish green, crimson (limit 50 .gamma./cc.); naphthoimidazole, yellow, reddish orange (limit 100 .gamma./cc.); quinazoline, blood-red, blood-red; **quinoxaline**, blood-red, reddish violet; 1-(2-benzimidazolyl)1,2,3,4,5-pentahydroxypentane, yellow, light yellow; 1-(2-quinoxalinyl)-1,2,3,4-tetrahydroxybutane, yellow, light yellow; 2-methylbenzothiazole-EtI, bluish green, violet; 2-ethylbenzothiazole-EtI, yellow, reddish brown; quinaldine-EtI, green, bluish violet; lepidine-EtI, green, bluish violet; 2,4-dimethylthiazole-EtI, blood-red, violet; benzoxazole-EtI, yellow, light yellow; 2-adeninethiol, yellowish brown, green; adenine, yellow, reddish violet; guanine, yellow, white ppt.; 8-azaguanine, yellow, white ppt.

L5 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS
AN 1952:54597 CAPLUS
DN 46:54597
OREF 46:9094h-i,9095a-h
TI Organic reactions in aqueous solution at room temperature. I. The influence of pH on condensations involving the linking of carbon to nitrogen and of carbon to carbon
AU Haley, C. A. C.; Maitland, P.
CS Univ. Cambridge, UK
SO J. Chem. Soc. (1951) 3155-74
DT Journal
LA Unavailable
IT **5122-36-1**, Formamide, N-(4,6-diamino-5-pyrimidinyl)- (prepn. of)
RN 5122-36-1 CAPLUS
CN Formamide, N-(4,6-diamino-5-pyrimidinyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



AB The object of this series of papers is to broaden the field initiated by Robinson and Schopf and usually termed "syntheses under physiol. (or cell-possible) conditions" in relation to both biochem. problems and general org. synthetical methods. Extensive (rather than intensive) investigations have shown that H2O at room temp. is an effective medium for some very simple condensations involving substances contg. the naturally occurring groups CHO, CO, NH2, CONH2, NH2C:NH, CH2CN, CH2CO, COCH2CO, COCH2CH2CO (and HCO2H), leading to well-known examples of Schiff bases, and **quinoxaline**, diazepine, pyrimidine, glyoxaline, pyrrole, and pyridine derivs. Some failures have suggested that in this type of work, a CH2 group requires activation from both sides for successful condensation. In 2 cases of Claisen-Knoevenagel condensations, glycine is a useful catalyst. As found by Schopf in other cases, variation of the pH has striking effects on the yields. The reaction conditions differed from those used by Robinson and Schopf in that, whereas they usually had to isolate their products from soln., H. and M. chose H2O-sol. reactants which produced very difficultly sol. products. A

considerable part of the driving force for the reactions is therefore the displacement of equil. by pptn. The products in most cases are obtained in reasonable, and sometimes very high, yields after a reaction time of a few days, and are isolated in pure form directly from the reaction mixt., the usual losses thus being eliminated. Several of the reactions may have preparative value or may serve for future kinetic investigations. Some of the exptl. results support the theory that some reactions, normally considered to be base-catalyzed, may also take place under acid conditions. The following solubilities in H2O at approx. 18.degree. (g./100 g.) are reported: p-MeOC6H4CHO 0.38, p-HOC6H4CHO 0.81, PhCH:CHCHO 0.14, 1-C10H7CHO 0.14, o-C6H4(NH2)2 (I) 2.16. Details are given (in tables) of the following reactions at various pH (time at room temp. given). PhCH:NPh from BzH and PhNH2 (2 days): 80% at pH 7-7.9, 0% at pH 3.8. 2,3-Dimethylquinoxaline from I and Ac2 (1 day): 81-98% at pH 4-9, 44% at pH 3, 82% at pH 11.6. 5,7-Dimethyl-2,3-benzo-1,4-diazepine from I and CH2Ac2 (2 hrs.): 56% at pH 5.8, 0% at pH 8.2; HCl salt ppts. at pH 3.8. 2-Amino-4,6-dimethylpyrimidine from (H2N)2C:NH.H2CO3 and CH2Ac2 (20 days): 62% at pH 10, 0% at pH 8.5. 4,6-Dimethyl-2-phenylpyrimidine from PhC(:NH)NH2 (19 days): 64% at pH 9.6, 36% at pH 9.1, 26% at pH 8.9, 8% at pH 8.7, 0% at pH 7.5 or below. Benzimidazole from I and HCO2H (5 days): 83% at pH 0.5, 25% at pH 2.3, 0% at pH 3.3. 4,6-Diamino-5-formamidopyrimidine (II) from 4,5,6-triaminopyrimidine (III) and HCO2H (4 days): 61% at pH 1.1, 3% at pH 2.8 or 0.3, 0% at 3.0 or above; adenine could not be detected but was formed by heating II 4 hrs. at 230.degree.; II was not cyclized (7 days at room temp.) at pH 11 or above (at pH 14 III was regenerated). (Furfurylideneacetyl)acetone (IV), m. 55-7.degree., at pH 4 results in 17% yield from furfuraldehyde (V) and CH2Ac2 in 3 days and in 67% yield after 14 days; IV results (6 days) in 60-76% yield in the pH range 3.6-6.5; in the presence of 2 g. glycine (0.96 g. V), the yield is 92% (pH 4.7 (17% without catalyst); 0.1 g. glycine gives 56% and 1 g. gives 83%. 4-Cyanomethylimino-2-pentanone, m. 112-13.degree. (from H2NCH2CN and CH2Ac2)(8 days) results in 67-9% yields at pH 6.9-8.0; HO2CCH2N:CMeCH2Ac (from H2NCH2CO2Et and CH2Ac2)(2 days) is formed in 46-8% yield at pH 8.3-8.7, 0% at pH 7.1 or 9.0. 1-Benzyl-2,5-dimethylpyrrole (from PhCH2NH2 and CH2Ac2)(7 days) results in 68-70% yield at pH 10.9-11.5, 1% at pH 7.1, and 0% at pH 5.8 or below. 2,5-Dimethyl-1-phenylpyrrole (from PhNH2 and CH2Ac2)(8 days) results in 70% yield at pH 4.4 or 5.5, 0% above pH 8.2. Et 2-methyl-4-phenyl-3-pyrrolecarboxylate (from BzCH2NH2 and AcCH2CO2Et)(3 days) results in 63% yield at pH 6.9-8.2, 14% at pH 6.1, and 2% at pH 3.9. 3-Cyano-4,6-dimethyl-2-pyridone (from NCCH2CONH2 and CH2Ac2)(1 day) results in 74% yield at pH 9.1 and 20% at pH 6.4; in another expt., with K2CO3 (1 day), the yield was 94-6% at pH 8.5-9.1, 0% at pH 4.4, 20% at pH 6.4. Di-Et 1,4-dihydrocollidine-3,5-dicarboxylate (from AcH, AcCH2CO2Et, and NH3) (4 days) results in 43% yield at pH 8.5 and 3% at pH 6. 3,5-Diacetyl-1,4-dihydrocollidine (from AcH, CH2Ac2, and NH3) (4 days) is formed in 23-9% yield at pH 6.3-9.0; with (NH4)2CO3 the reaction is slower but the yield at pH 8.1 is 51%.

=> d cost

COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
CONNECT CHARGES	1.36	1.85
NETWORK CHARGES	0.24	0.36
SEARCH CHARGES	1.64	149.39
DISPLAY CHARGES	43.20	43.20
	46.44	194.80

CAPLUS FEE (5%)	2.31	2.31
FULL ESTIMATED COST	48.75	197.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.51	-6.51

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